STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 109892

TO: Deborah Lambkin
Location:
Art Unit: 1626
December 5, 2003

Case Serial Number: 09/496695

From: P. Sheppard
Location: CM1-1E03
Phone: (703) 308-4499

sheppard@uspto.gov

Search Notes

Access DB# 109897

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Deborah Lambkin Examiner #: 71320 Date: 11/25/03
Art Unit: 1616 Phone Number 30 8-4522 Serial Number 09/496,695
Mail Box and Bldg/Room Location: CM1 3C23 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Substituted Benzopyran Der.

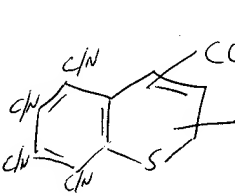
Inventors (please provide full names): _____

_____

Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

R + R, important.



COOH, COO^- alkyl, $\overset{\oplus}{E}-N<$

Cl, NO_2, CN, halo, alkoxy

see data attached.

Thanks

STAFF USE ONLY

Searcher: Stephanie

Searcher Phone #: 308-4499

Type of Search

NA Sequence (#)_____

AA Sequence (#)_____

Vendors and cost where applicable

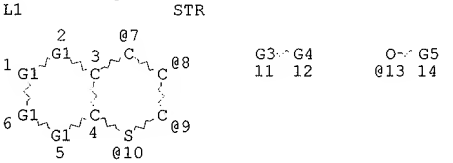
STN _____

Dialog _____

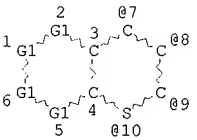
```
=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 18:37:51 ON 05 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)
```

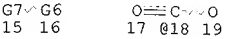


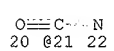
```
FILE COVERS 1907 - 5 Dec 2003  VOL 139 ISS 24
FILE LAST UPDATED: 4 Dec 2003  (20031204/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=>
=>

=> d stat que
L1                  STR
```




```
VAR G1=C/N
VAR G3=7/8/9/10
VAR G4=X/NO2/CN/13
VAR G5=ME/ET/I-PR/N-PR/I-BU/T-BU/S-BU/N-BU
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14

STEREO ATTRIBUTES: NONE
L2          1394 SEA FILE=REGISTRY SSS FUL L1
L7                  STR
```







VAR G1=C/N
VAR G6=18/21
VAR G7=7/8/9/10
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L9 1704 SEA FILE=REGISTRY SSS FUL L7
L10 24 SEA FILE=REGISTRY ABB=ON PLU=ON L9 AND L2
L14 13 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

=>
=>

=> d ibib abs hitrn l14 1-13

L14 ANSWER 1 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:106551 HCAPLUS
DOCUMENT NUMBER: 116:106551
TITLE: Synthesis of 20-alkyl-8-thiathevinols, opiate agonists derived from 8-thiathevinone, the cycloadduct of thebaine and 2-oxopropanethial
AUTHOR(S): Kirby, Gordon W.; Sclare, Alastair D.
CORPORATE SOURCE: Dep. Chem., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1991), (10), 2329-38
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 116:106551
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The cycloadduct I was prepd. from thebaine (II) and the transient thioaldehyde EtO2CCHS formed in situ from the Bunte salt EtO2CCH2SSO3Na. The thermal isomerisation of I to give the regioisomer III was reinvestigated. Prolonged heating gave an equil. mixt. of III and the

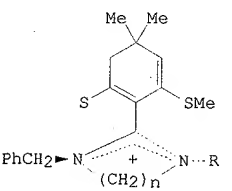
major, rearrangement product IV. Base catalyzed epimerization of I gave the 7.beta.-isomer. II and 2-oxopropanethial gave the cycloadduct 8-thiathevinone V. V was converted with Grignard reagents into a series of (20R)- and (20S)-20-alkyl-8-thiathevinols VI (R = alkyl). The reactions were not stereoselective. The analgesic potency, in guinea-pig ileum prepns., of the alkylthiathevinols VI depended upon the C-20 configuration and the alkyl chain length. The (20R)-epimers were the more potent, the max. potency being obsd. for the (20R)-20-pentyl deriv., which was equipotent with N-normorphine. Generally, the thiathevinols were much less potent than the corresponding thevinols.

IT **87817-36-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and isomerization of)

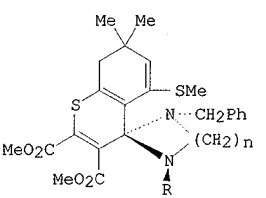
IT **138916-18-4P 138916-19-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **139066-01-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., Grignard methylation, and epimerization of)

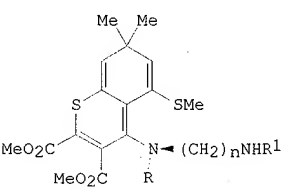
L14 ANSWER 2 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:449581 HCAPLUS
DOCUMENT NUMBER: 115:49581
TITLE: Addition of twisted 1-thioacyl-2,2-diaminoethylenes to dimethyl acetylenedicarboxylate. Formation and ring opening of thiopyran-4-spiro-2'-(1',3'-diazacyclanes)
AUTHOR(S): Khan, Agha Zul Qarnain; Sandstroem, Jan
CORPORATE SOURCE: Chem. Cent., Univ. Lund, Lund, S-221 00, Swed.
SOURCE: Journal of Organic Chemistry (1991), 56(5), 1902-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:49581
GI



I



II

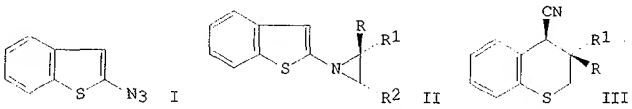


III

be eventually produced, in competition with unimol. ring cleavage fragmentation leading to the enethione III, probably via concerted ring opening and nitrogen extrusion. Suitable support has been provided by the finding that 3-azidobenzo[b]thiophene can exhibit analogous cycloaddn. reactions with alkenes under the same reaction conditions. The present evidence contradicts a previous claim (Spagnolo, P.; Zanirato, P., 1985, 1988) that a singlet nitrene should be an intermediate in the formation of aziridine and ring cleavage products arising from decompn. of I in the presence of alkenes.

IT **120810-24-4P 132681-55-1P 132681-56-2P**
132681-57-3P 132747-92-3P 132747-93-4P
132747-94-5P 132747-95-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 4 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1989:230939 HCAPLUS
DOCUMENT NUMBER: 110:230939
TITLE: Thermal fragmentation of 2-azidobenzo[b]thiophene in the presence of alkenes: a new synthetic route to 1-(2-benzo[b]thienyl)aziridines and/or thiochroman-4-carbonitriles
AUTHOR(S): Spagnolo, Piero; Zanirato, Paolo
CORPORATE SOURCE: Ist. Chim., Univ. Basilicata, Potenza, 85100, Italy
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (12), 3375-80
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:230939
GI



AB Mild thermal fragmentation of 2-azidobenzo[b]thiophene (I) in the presence of the olefins results in the formation of (benzo[b]thienyl)aziridines (II; R, R1 = H, alkyl; R2 = H, alkyl, Cl, CN, CO2Me) and/or 4-cyanothiochromans (III; R = H, alkyl; R1 = H, alkyl, Cl, CN, CO2Me) in fairly good yields. The formation of aziridines, at the expense of thiochromans, is favored by electron-poor olefins and by a decrease in the reaction temp. Evidence is presented in favor of a singlet nitrene intermediate which adds to the olefin double bond or undergoes a ring-opening reaction to give an o-quinoidal enethione which is trapped by the alkene present. These findings provide the first example of ready ring opening by a 2-nitreno-substituted thiophene.

IT **120810-24-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 5 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1987:423538 HCAPLUS
DOCUMENT NUMBER: 107:23538
TITLE: Preparation and chemistry of the Diels-Alder adducts of levopimaric acid and activated thiocarbonyl

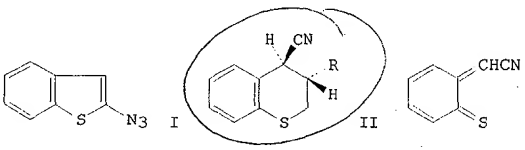
AB Reaction of 1,3-dialkyl-2-(4,4-dimethyl-2,6-dithioxocyclohexylidene)imidazolidines and -hexahydropyrimidines (twisted push-pull ethylenes with Me iodide followed by treatment with base leads smoothly to S-Me derivs., which are betaines with a 1,4-dipole and an electron-rich 1,3-butadiene system I (R = PhCH2, Me2CH, n = 2, 3). These compds. react with MeO2CC.tplbond.CCO2Me to give dihydrobenzothiopyranspiroimidazolidine and -hexahydropyrimidine derivs. II in high yields. The spiro compds. rearrange in acid medium or on chromatog. on silica gel to compds., which we previously incorrectly described as "folded ethylenes" but which are now shown to be 4-(1-aminoethyl)amino- or 4-(3-aminopropyl)aminothiopyran derivs. III (R, R2 = PhCH2, Me2CH). The 4-amino groups of III are twisted out of the thiopyran plane by the flanking substituents, and the barrier to rotation through the plane was found by NMR bandshape anal. to be 17.8 kcal/mol for the (2-aminoethyl)amino and 16.9 kcal/mol for the (3-aminopropyl)amino group. A 1:2 adduct of I and MeO2CC.tplbond.CCO2Me which we also previously incorrectly described as a folded ethylene, was shown to be an aminomaleic ester deriv. formed by addn. of the NH group of II to DMAD.

IT **132206-27-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and NMR of)

L14 ANSWER 3 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN

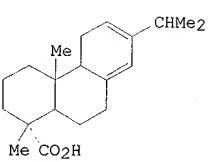
ACCESSION NUMBER:	1991:143072 HCAPLUS
DOCUMENT NUMBER:	114:143072
TITLE:	Thermal reactivity of 2-azido- and 3-azido-benzo[b]thiophene with alkenes
AUTHOR(S):	Funicello, Maria; Spangnolo, Piero; Zanirato, Paolo
CORPORATE SOURCE:	Ist. Chim., Univ. Basilicata, Potenza, 85100, Italy
SOURCE:	Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1990), (11), 2971-8 CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 114:143072

GI

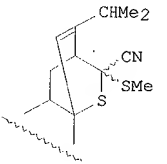


AB Thermal decompn. of 2-azidobenzo[b]thiophene (I) in the presence of various (E)- and (Z)-alkenes, at room temp., affords thiochroman-4-carbonitriles II (R = H, CN, CO2Me), resulting from cycloaddn. of an o-quinoidal enethione intermediate III to the olefin double bonds, and 1-(2-benzothienyl)aziridines which generally occur in a nonstereospecific fashion. In one case, i.e., with di-Et fumarate, clear-cut spectroscopic and chem. evidence for the intermediacy of a triazoline adduct in the formation of the obsd. trans- and cis-aziridines has been obtained. In the presence of 1-pyrrolidinylcyclopentene or -cyclohexene, the azide furnishes an isolated triazoline in quant. yield, whereas Me (E)-3-(N-pyrrolidinyl)acrylate leads to Me 1-(2-benzothienyl)triazole-4-carboxylate, arising from an intermediate triazoline by readily occurring elimination of pyrrolidine. Results suggest that I generally undergoes cycloaddn. reactions to give triazoline adducts, from which aziridines can

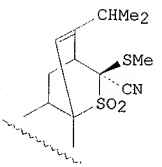
dienophiles
AUTHOR(S): Friedrich, Joyce D.
CORPORATE SOURCE: Dep. Chem., Univ. Alabama, Birmingham, AL, 35294, USA
SOURCE: Journal of Organic Chemistry (1987), 52(12), 2442-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 107:23538
GI



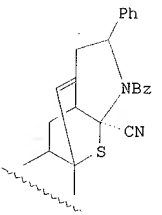
I



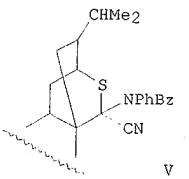
II



III



IV

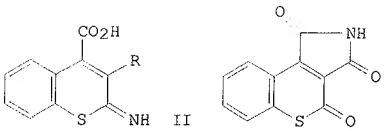


V

AB Treating levopimaric acid (I) with NCCS2Me gave 93% of a mixt. contg. 37% endo CN and 56% endo MeS II; the latter was oxidized by KMnO4 followed by treatment with NH2OH.cntdot.HCl to give sulfone III. Treating I with BzN(CSCN)Ph gave thiopyranopyridine IV and the thiopyran V. Hydrogenation and hydrolysis reactions of the various products were studied.

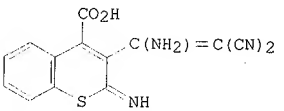
IT **108214-21-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 6 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:50757 HCAPLUS
DOCUMENT NUMBER: 104:50757
TITLE: Reactions with benzo[b]thiophene-2,3-dione. A novel synthesis of thiocoumarin derivatives
AUTHOR(S): Sallam, Mohamed Mohamed Mohamed; Ibraheim, Mahmoud Ali; Elnagdi, Mohamed Hilmy; Sadek, Kamal Usef
CORPORATE SOURCE: Fac. Sci., Cairo Univ., Giza, Egypt
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1985), 327(2), 333-6
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:50757
GI

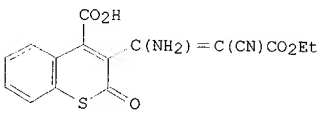


II

III



IV



V

AB Condensation of the title dione (I) with RCH2CN (R = cyano, CO2Et) in the presence of Et3N gave the benzothiopyrans II; the reaction of I with EtO2CCH2CN also yielded the imide III. Similar reaction of I with R1CH2C(NH2):CR1CN (R1 = cyano, CO2Et) gave benzothiopyrans IV and V.

IT **99875-39-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

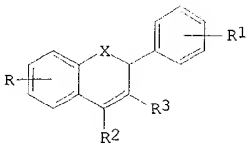
L14 ANSWER 7 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:50730 HCAPLUS
DOCUMENT NUMBER: 104:50730
TITLE: Pharmaceutical preparations containing flavene or thioflavene derivatives, their use, and flavenes and thioflavenes
INVENTOR(S): Rimbault, Christian Gerard; Narbel, Philippe Marcel
PATENT ASSIGNEE(S): Zyma S. A., Switz.
SOURCE: Brit. UK Pat. Appl., 35 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2145720	A1	19850403	GB 1984-21778	19840829
GB 2145720	B2	19870204		
US 4665202	A	19870512	US 1984-644006	19840824
FI 8403364	A	19850301	FI 1984-3364	19840827
FI 83780	B	19910515		
FI 83780	C	19910826		
EP 140830	A2	19850508	EP 1984-810424	19840827
EP 140830	A3	19860108		
EP 140830	B1	19890830		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
AT 45878	E	19890915	AT 1984-810424	19840827

IL 72776	A1	19910131	IL 1984-72776	19840827
DD 222025	A5	19850508	DD 1984-266736	19840829
CA 1247615	A1	19881227	CA 1984-462008	19840829
NO 8403455	A	19850301	NO 1984-3455	19840830
DK 8404161	A	19850301	DK 1984-4161	19840830
ZA 8406786	A	19850424	ZA 1984-6786	19840830
HU 36819	A2	19851028	HU 1984-3262	19840830
AU 8432572	A1	19860911	AU 1984-32572	19840830
AU 577308	B2	19880922		
JP 60149581	A2	19850807	JP 1984-180892	19840831
ES 535590	A1	19880501	ES 1984-535590	19840831

PRIORITY APPLN. INFO.: GB 1983-23293 19830831
EP 1984-810424 19840827

OTHER SOURCE(S): CASREACT 104:50730
GI



I

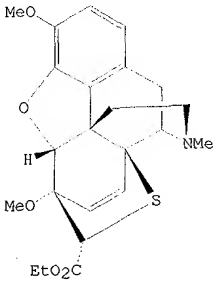
AB Title compds. I [R, R1 = H, OH, alkoxy, alkanoyloxy, SH, alkylthio, (un)substituted amino, alkyl, halo, carboxy, alkoxycarbonyl, carbamoyl, cyano, NO2, amidated sulfo, etc.; R2, R3 = H, halo, (un)substituted amino, a quaternary ammonium salt, OH, SH, NO2, formyl, carboxy, aryl, alkyl, heterocyclyl, etc.; X = O, S, SO, SO2) and their salts, useful as mucolytics, immunostimulants, and for the treatment of liver diseases (no data), were prepd. Thus, treating 4-chloro-3-formylflav-3-ene with NaOMe in MeOH gave I (R = R1 = H, R2 = MeO, R3 = CHO).

IT **99943-65-4P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)

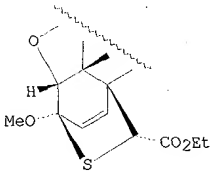
L14 ANSWER 8 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:	1986:5547 HCAPLUS
DOCUMENT NUMBER:	104:5547
TITLE:	Ethyl and methyl thioxoacetates, dienophilic thioaldehydes formed from sulfenyl chlorides by 1,2-elimination
AUTHOR(S):	Bladon, Christine M.; Ferguson, Irene E. G.; Kirby, Gordon W.; Lochead, Alistair W.; McDougall, Duncan C.
CORPORATE SOURCE:	Dep. Chem., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE:	Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1985), (7), 1541-5 CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE:	Journal
LANGUAGE:	English
OTHER SOURCE(S):	CASREACT 104:5547

GI



III

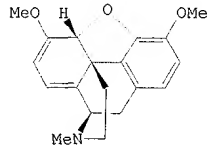


IV

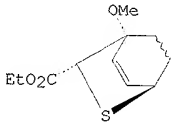
AB Treatment of RO2CCH2SCl (I; R = Me, Et) with Et3N at room temp. gave the corresponding RO2CCHS (II). Generation of transient II (R = Et) in the presence of conjugated dienes gave the corresponding cycloadducts. E.g., treatment of I (R = Et) with Et3N in C6H6-MeOH contg. thebaine at room temp. gave 67% cycloadduct III, which isomerized at 111.degree. to the more stable adduct IV by dissocn. and recombination. Cycloadducts of II (R = Et) and anthracene or 9,10-dimethylanthracene similarly dissocd. at 111.degree., providing a clean and convenient source of II (R = Et).

IT **87817-36-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)

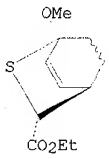
L14 ANSWER 9 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1983:557787 HCAPLUS
DOCUMENT NUMBER: 99:157787
TITLE: Generation of ethyl thioxoacetate, a dienophilic thioaldehyde
AUTHOR(S): Bladon, Christine M.; Ferguson, Irene E. G.; Kirby, Gordon W.; Lochead, Alistair W.; McDougall, Duncan C.
CORPORATE SOURCE: Dep. Chem., Univ. Glasgow, Glasgow, G12 8QQ, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1983), (8), 423-5
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



II



III



IV

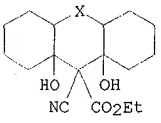
AB Reaction of EtO2CCH2SCl (I) with Et3N gave the transient thio aldehyde EtO2CCHS which was trapped by cycloaddn. with conjugated dienes. E.g., reaction of I with thebaine II in C6H6 contg. Et3N at room temp. for 0.5 h gave the kinetic adduct III, which on refluxing in PhMe for 8 h gave the thermodn. adduct IV.

IT **87817-36-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and rearrangement of)

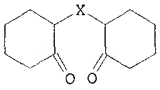
L14 ANSWER 10 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER:	1979:137783 HCAPLUS
DOCUMENT NUMBER:	90:137783
TITLE:	Reaction of 1,5-diketones with ethylcyanoacetate
AUTHOR(S):	Usol'tsev, A. A.; Karaulov, E. S.; Tilichenko, M. N.
CORPORATE SOURCE:	Dal'nevost. Gos. Univ., Vladivostok, USSR
SOURCE:	Zhurnal Organicheskoi Khimii (1978), 14(11), 2458-9 CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE:	Journal
LANGUAGE:	Russian

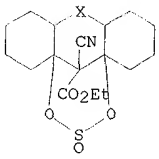
GI



I



II



III

AB Tricyclic esters I (X = CH2, S), obtained in 23 and 82% yields by cycloaddn. of EtO2CCH2CN to cyclohexanones II, were cyclized by SOCl2 to give cyclic sulfites III.

IT **69695-02-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and cyclic sulfite formation from)

IT **69695-03-0P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 11 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:592270 HCAPLUS
DOCUMENT NUMBER: 83:192270
TITLE: Rearrangement of 10-bromo-10,11-dihydrodibenzo[b,f]thiepin-11-one and related compounds in an alkaline solution
AUTHOR(S): Ueda, Ikuo
CORPORATE SOURCE: Res. Lab., Fujisawa Pharm. Co., Ltd., Osaka, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1975), 48(8), 2306-9
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The reaction of 10-bromo-10,11-dihydrodibenzo[b,f]thiepin-11-one (I) with NaOMe in MeOH leads to thioxanthone (II) and 10-hydroxy-10,11-dihydrodibenzo[b,f]thiepin-11-one (III). If the reaction of I is carried out in an aq. sodium hydroxide soln., six products II, III, 9-hydroxythioxanthene-9-carboxylic acid, thioxanthene-9-carboxylic acid, thioxanthene, and 10,11-dihydrodibenzo[b,f]thiepin-10-one, are formed. The mechanism is discussed.
IT **57117-06-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 12 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1973:478739 HCAPLUS
DOCUMENT NUMBER: 79:78739
TITLE: Neurotropic and psychotropic agents. LVIII. 8-Hydroxy-10-(4-methylpiperazino)-10,11-dihydrodibenzo(b,f)thiepin, O-substitution derivatives, and some related compounds
AUTHOR(S): Sindelar, K.; Kakac, B.; Svatek, E.; Metysova, J.; Protiva, M.
CORPORATE SOURCE: Res. Inst. Pharm. Biochem., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1973), 38(5), 1579-95
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Demethylation of 8-methoxydibenzo[b,f]thiepin-10(11H)-one (I, R = Me) with C5H5N.HCl gave the 8-hydroxy analog (I, R = H) which was O-alkylated with EtI, BuBr, PhCH2Cl, and 2-bromopyridine giving the corresponding I. These were transformed in 3 steps to the 8-ethoxy (II), 8-butoxy (III), 8-benzyloxy (IV), and 8-(2-pyridyloxy) (V) derivs. of 10-(4-methylpiperazino)-10,11-dihydrodibenzo[b,f]thiepin. Debenzylation of IV with Na in BuOH led to the aminophenol VI. This resulted also from demethylation of 8-methoxy-10-chloro-10,11-dihydrodibenzo[b,f]thiepin with BBr3, a subsequent substitution reaction with 1-methylpiperazine and hydrolysis, and from reaction of 8-bromo-10-(4-methylpiperazino)-10,11-dihydrodibenzo[b,f]thiepin with Mg and by oxidn. of the Grignard reagent formed with air. Products obtained in the reaction of 8-methoxy-11-bromodibenzo[b,f]thiepin-10(11H)-one with 1-methylpiperazine were also studied.
IT **43183-19-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

L14 ANSWER 13 OF 13 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1968:29676 HCAPLUS
DOCUMENT NUMBER: 68:29676
TITLE: Neurotropic and psychotropic substances. XVII. 10-(4-Methylpiperazino)-1/,11-dihydrodibenzo(b,f)thiepin and analogs
AUTHOR(S): Jilek, Jiri O.; Svatek, Emil; Metysova, Jirina; Pomykacek, Josef; Protiva, Miroslav
CORPORATE SOURCE: Pharm. Res. Inst., Prague, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1967), 32, 3186-212
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The very high central depressant activity of the title compd. I (R = H) stimulated a study of structural analogs. 2-PhSC6H4CO2H reduced with LiAlH4 gave 82-93% 2-PhSC6H4CH2OH, m. 44.degree. (Et2O-petroleum ether). 10,11-Dihydrodibenzo[b,f]thiepin-10-ol (25 g.) in 200 ml. C6H6 satd. with anhyd. HCl and the mixt. dried with 10 g. anhyd. CaCl2, kept overnight at room temp., filtered, and evapd. gave 26.2 g. 10-chloro-10,11-dihydrodibenzo[b,f]thiepin (II), m. 84-4.5.degree. (cyclohexane). II (20 g.) and 40 ml. 1-(ethoxycarbonyl)piperazine (b18 125.degree.) heated 4 hrs. to 105.degree., the mixt. cooled, dild. with 200 ml. H2O, and extd. with 200 ml. C6H6, the ext. shaken with 120 ml. 3N HCl, and the sepd. HCl salt and the aq. soln. made alk. with 20% NaOH, and extd. with C6H6 gave 22.2 g. I (R = CO2Et) (III), m. 112-14.degree. (EtOH), H maleate m. 192-3.degree. (90% EtOH), mesylate m. 211-12.degree. (Me2CO-EtOH-Et2O). III (9.5 g.), 50 ml. HO(CH2)2OH, 5 g. KOH, and 5 ml. H2O refluxed 20 hrs., the mixt. cooled, dild. with H2O, and extd. with C6H6, the ext. shaken with 3N HCl, and the sepd. HCl salt filtered, treated with NH4OH, and extd. with C6H6 gave 7.3 g. I (R = H) (IV), m. 108.degree. (Me2CO). III (5 g.) hydrolyzed with 2.5 g. KOH in 5 ml. EtOH under reflux 2.5 hrs. at 120-5.degree. gave 4 g. IV, m. 105-7.degree., maleate m. 188-90.degree. (aq. EtOH). A mixt. of 6 g. IV and 40 ml. HCO2Et heated in a sealed tube 3 hrs. to 120.degree., cooled, and evapd., and the residue recrystd. from MeOH gave 5.4 g. I (R = CHO) (V), m. 135-6.degree. (EtOH), H maleate m. 162-4.degree. (EtOH). IV (2.5 g.) and 20 ml. 100% HCO2H refluxed 6 hrs., the mixt. evapd., the residue extd. with C6H6, and the ext. washed with dil. HCl gave 1.8 g. dibenzo[b,f]thiepin (VI), m. 88.degree. (EtOH). V (1.3 g.) reduced with 0.6 g. LiAlH4 in 40 ml. Et2O and 15 ml. tetrahydrofuran gave 0.9 g. I (R = Me) (VII), m. 134-5.degree. (MeOH), maleate m. 157-8.degree. (EtOH), fumarate, m. 199-201.degree. (aq. EtOH), monomethiodide m. 220-2.degree. (H2O). 10,11-Dihydrodibenzo[b,f]thiepin-10-one (VIII) (3 g.), 5 g. 1-methylpiperazine, and 5 g. 100% HCO2H heated 1 hr. to 180-90.degree. under reflux, and evapd. slowly during 8 hrs. at the same temp. gave 65 mg. VII, m. 134-5.degree.. VII (15.5 g.) and 9 g. dibenzoyl(+)-tartaric acid in 230 ml. EtOH gave 11.8 g. (+)-VII bis(hydrogendibenzoyl-(+)-tartrate), monohydrate m. 149-52.degree. (MeOH), [.alpha.]20D -30.degree.. Decompn. of 11 g. of the salt with NH4OH and extn. with C6H6 gave 6.9 g. (+)-VII, m. 106-7.degree. (MeOH), [.alpha.]20D 28.degree.; maleate m. 160-4.degree. (EtOH), [.alpha.]20D 30.degree.. A similar resoln. of (.+-.)-VII (2.4 g.) by means of 3 g. di-p-toluoyl-(-)-tartaric acid in EtOH gave 3.42 g. (-)-VII di-p-toluoyl-(-)-tartrate (m. 180-1.degree., [.alpha.20D 82.degree.) and impure (-)-VII, m. 105-8.degree. (MeOH), [.alpha.]20D -10.degree.. IV (3 g.) and 2 g. Na2CO3 in 60 ml. C6H6, stirred and treated with 1.5 g. AcCl in 10 ml. C6H6, the mixt. stirred 3 hrs. at room temp., refluxed 6 hrs., and decompd. with H2O gave 2.5 g. I (R = Ac) (IX), m. 129-31.degree. (MeOH). Treatment of 10 g. IV in 60 ml. AcOH with 10 g. Ac2O (refluxed 2 hrs.) gave 9 g. IX, m. 128-30.degree.. IX (12 g.) reduced with 4 g. LiAlH4 in 240 ml. Et2O and 120 ml. tetrahydrofuran gave I (R = Et) (X), m. 85-6.degree. (petroleum ether), maleate (9.1 g.) m. 150-1.degree. (EtOHEt2O). IV (16.5 g.) in 11.5 ml. H2O treated with 16.5 ml. dild. 1:1

HCl, the soln. treated in 30 min. with 5.5 g. NaNO2 in 16 ml. H2O at 75-80.degree., the mixt. stirred 2 hrs. at 80.degree., kept overnight, dild. with H2O, neutralized with Na2CO3, and extd. with Et2O gave 13.4 g. I (R = NO) (XI), m. 128-9.degree. (EtOH). XI (9.8 g.) reduced with 3 g. LiAlH4 in 330 ml. tetrahydrofuran gave 8.6 g. I (R = NH2), m. 157-8.degree. (cyclohexane-EtOH), maleate m. 167-8.degree. (EtOH-Et2O). II (12 g.) and 20.8 g. 1-(2-hydroxyethyl)piperazine (b15 120.degree.) heated 4 hrs. to 110.degree. and the mixt. cooled, and dild. with H2O gave 9.65 g. I (R = (CH2)2OH) (XII), m. 108-10.degree. (aq. EtOH), maleate m. 129-30.degree. (EtOH-Et2O). II (9 g.) and 15 g. 1-(3-hydroxypropyl)piperazine (b10 136-40.degree.) heated 2.5 hrs. to 110-25.degree. gave similarly 7.7 g. I [R = (CH2)3OH) (XIII), m. 138.degree. (aq. EtOH), maleate m. 156.degree. (EtOH). Treatment of 2.5 g. XIII in 10 ml. C6H6 and 5 ml. CHCl3 with 2.5 ml. AcCl at room temp.- gave 2.07 g. I [R = (CH2)3OAc] (XIV), bis(hydrogen maleate) m. 137-8.degree. (aq. Me2CO). II (12 g.) and 24 ml. 1-phenylpiperazine (b10 149-58.degree.) heated 3.5 hrs. to 125-30.degree. gave 14 g. I (R = Ph), m. 185-6.degree. (C6H6-EtOH), mesylate m. 213-14.degree. (EtOH). II (12 g.) and 24 ml. 1-benzylpiperazine (b0.4 90.degree.) gave similarly 15.5 g. I (R = CH2Ph), m. 148-9.degree. (EtOH-C6H6), maleate m. 210-11.degree. (EtOH-C6H6). II (9 g.) and 15 g. 1-methylhexahydro-1,4-diazepine (b60 85.degree.) heated 3.5 hrs. to 105.degree. gave 7.6 g. 10-(4-methylhexahydro-1,4-diazepino)-10,11-dihydrodibenzo[b,f]thiepin, m. 82.degree. (petroleum ether), maleate m. 142.degree. (EtOH). A similar reaction with 4-hydroxypiperidine (b20 118-22.degree., b11 112.degree.) gave 78% 10-(4-hydroxypiperidino)-10,11-dihydrodibenzo[b,f]thiepin, m. 145-6.degree. (EtOH), H maleate m. 173-4.degree. (EtOH-Et2O). 1-Methyl-4-chloropiperidine (12.15 g., b25 70.degree.) treated with 2.2 g. Mg in 65 ml. tetrahydrofuran, the Grignard reagent treated dropwise with 10 g. II in 35 ml. tetrahydrofuran, and the mixt. stirred 2.5 hrs. at room temp., kept overnight, refluxed 2 hrs., cooled, decompd. with 15% NH4Cl, and extd. with Et2O gave 3.3 g. 10-(1-methyl-4-piperidyl)-10,11-dehydrodibenzo[b,f]thiepin (XV), H maleate m. 159.5-60.5.degree. (EtOH) HCl salt of VII (from 2 g. VII) in 20 ml. MeOH and 15 ml. H2O stirred and treated with NaIO4 (prepd. from 1.5 g. H5IO6) in 15 ml. H2O, the mixt. kept 24 hrs. at room temp., and evapd. in vacuo, the residue dild. with H2O, treated with NH4OH, and extd. with C6H6, and the crude product sepd. from neutral impurities and chromatographed on neutral Al2O3 gave 10-(4-methylpiperazino)-10,11-dihydrodibenzo[b,f]thiepin 5-oxide, maleate (0.53 g.) m. 165-7.degree. (EtOH-Et2O), maleate solvated with EtOH m. 135-40.degree. (EtOH-Et2O). Oxidn. of VII (2 g.) with 35% H2O2 (10 ml.) in 25 ml. AcOH refluxed 2 hrs. resulted in cleavage of the mol. and gave 1.1 g. dibenzo[b,f]thiepin 5,5-dioxide (XVI), m. 168-75.degree. (EtOH). Similar oxidn. of 2 g. III gave 0.85 g. XVI, m. 160-75.degree.. VI (2 g.) in 20 ml. AcOH and 15 ml. Me2CO oxidized similarly with 10 ml. 30% H2O2 gave 1.3 g. XVI, m. 175-80.degree. (EtOH). Oxidn. of 2 g. VII in 20 ml. AcOH with 4 ml. 30% H2O2 at room temp. (17 days of standing) gave 1.2 g. mol. complex of XVI and dibenzo[b,f]thiepin 5-oxide, m. 127-8.degree. (C6H6-petroleum ether or EtOH). VIII (2 g.) in 20 ml. Me2CO and 7 ml. AcOH stirred and treated dropwise with 4 ml. 30% H2O2, the mixt. kept overnight at room temp., refluxed 1 hr., evapd. in vacuo, and the residue dild. with H2O gave 1.2 g. 10,11-dihydrodibenzo[b,f]thiepin-10-one 5-oxide, m. 184-7.degree. (EtOH). VIII (1 g.) in 20 ml. 98% HCO2H treated with 2 ml. 30% H2O2, the mixt. kept overnight at room temp., heated 30 min. to 40.degree. and 4 hrs. to 90.degree., and dild. with H2O gave 0.95 g. 10,11-dihydrodibenzo[b,f]thiepin-10,11-dione 5,5-dioxide (XVII), m. 278-80.degree. (AcOH). XVII (0.25 g.) and 20 ml. 10% KOH heated 30 min. to 100.degree., the mixt. dild. with H2O, the solid filtered, heated 30 min. with 5 ml. 3N HCl to 100.degree., and cooled gave 0.12 g. thioxanthone 5,5-dioxide, m. 190-1.degree. (EtOH). 11-Methyl-10,11-dihydrodibenzo[b,f]thiepin-10-one (22.5 g.) in 400 ml. warm MeOH reduced with 7.5 g. NaBH4 in 20 ml. H2O and 30 ml. MeOH (with a trace of NaOH), the mixt. refluxed 2.5 hrs. and evapd., and the residue dild. with H2O,

and extd. with C6H6 gave 13 g. 11-methyl-10,11-dihydrodibenzo[b,f]thiepin-10-ol (XVIII), b0.8 178-85.degree.. XVIII (13 g.) in 100 ml. C6H6 treated with 3 g. anhyd. CaCl2 and satd. with anhyd. HCl, the mixt. kept overnight at room temp., filtered, and evapd., and the residue (13 g.) crystd. from Et2O at 0.degree. gave 4.55 g. 10-chloro-11-methyl-10,11-dihydrodibenzo[b,f]thiepin (XIX), m. 121-2.degree. (cyclohexane). XIX (4 g.) heated 2.5 hrs. with 8 ml. 1-methylpiperazine to 120-30.degree. gave 2.8 g. 10-(4-methylpiperazino)-11-methyl-10,11-dihydrodibenzo[b,f]thiepin, m. 119.degree. (petroleum ether), maleate m. 145-7.degree. (EtOH-Et2O). VIII (5 g.) in 200 ml. CHCl3 treated in 20 min. with 19 g. Br in 50 ml. CHCl3 and the mixt. stirred 2 hrs. at room temp., washed with H2O, dried, and evapd. gave 31.8 g. 11-bromo-10,11-dihydrodibenzo[b,f]thiepin-10-one (XX), m. 109-10.degree. (cyclohexane). XX (60.7 g.) in 500 ml. C6H6 treated with 60 g. 1-methylpiperazine, the mixt. kept 24 hrs. at room temp., refluxed 2 hrs., and the product sepd. into neutral and basic fractions gave 35 g. 11-(4-methylpiperazino)-10,11-dihydrodibenzo[b,f]thiepin-10-one (XXI), m. 68-70.degree.; maleate m. 153-5.degree. (EtOH). The neutral fraction (19.8 g.) from the foregoing expt. was sepd. by crystn. and chromatog. to give 3.02 g. VIII (m. 64-5.degree.) and 2 g. yellow 10,11-dihydrodibenzo[b,f]thiepin-10,11-dione (XXII), m. 135-6.degree. (cyclohexane). XXII (1.5 g.) and 100 ml. 10% NaOH heated 2 hrs. to 100.degree. and the mixt. cooled, dild. with H2O, and acidified with HCl gave 1.14 g. 9-hydroxythioxanthene-9-carboxylic acid (XXIII), monohydrate, m. 100-30.degree. and after resolidifying 190-220.degree. (AcOH). XXIII (prepd. from 0.9 g. XXII) dissolved in 5 ml. hot MeOH gave 0.67 g. 9-methoxythioxanthene-9-carboxylic acid, m. 205-8.degree. (MeOH). XXIII (0.35 g.) heated 1.5 hrs. to 150-60.degree. gave 90 mg. thioxanthone (XXIV), m. 210-15.degree. (AcOH). Treatment of 2 g. XXI with 3 ml. 80% N2H4 and 3 g. KOH in 20 ml. diethylene glycol 2 hrs. at 150-60.degree. and 4 hrs. at 180-200.degree. gave 1.3 g. neutral product which was recrystd. from EtOH giving 0.3 g. XXIV, m. 212-14.degree. (C6H6). XXI (5 g.) in 80 ml. EtOH reduced with 2 g. NaBH4 in 10 ml. 0.5N NaOH, the mixt. stirred and refluxed 2 hrs., evapd., and the residue dild. with H2O and extd. with C6H6 gave 3.75 g. 11-(4-methylpiperazino)-10,11-dihydrodibenzo[b,f]thiepin-10-ol (XXV), m. 148-52.degree. (EtOH), maleate m. 171.degree. (EtOH), 2HCl salt monohydrate m. 185-90.degree. (aq. EtOH). III (10 g.), 50 ml. AcOH and 20 ml. HBr refluxed 6 hrs., the mixt. cooled, dild. with 200 ml. H2O, made alk. with NH4OH, and extd. with C6H6, the ext. evapd., and the oily residue (6 g., contg. VI) crystd. from 10 ml. cyclohexane gave 0.6 g. 10,10'-bi(dibenzo[b,f]thiepin) (XXVI), yellow prisms of m. 277.degree. (PhMe). XXV (2 g.) and 3 g. 4-MeC6H4SO3H heated 1 hr. to 150.degree. and the neutral product (0.93 g.) recrystd. from C6H6 gave 0.35 g. XXVI, m. 272-7.degree.. VI (4 g.) in 70 ml. EtOH treated with 4 g. Na in 20 min. gave 2.1 g. dihydro compd., b0.1 125-30.degree., not crystg. on inoculation with authentic 10,11-dihydrodibenzo[b,f]thiepin (Jilek, et al., CA 63: 2952f). VI (3 g.), 20 ml. AcOH, 10 ml. 56% HI, and 1.5 g. P refluxed 2.5 hrs. gave quant. 9-methylthioxanthene, m. 83.degree. (petroleum ether or EtOH). VI (12.6 g.) in 100 ml. Et2O treated with 9.6 g. Br in 10 ml. CHCl3 and the mixt. stirred 2 hrs. at room temp. and kept at 0.degree. gave 19.5 g. 10,11-dibromo-10,11-dihydrodibenzo[b,f]thiepin (XXVII), m. 144-6.degree. (C6H6). XXVII (5 g.), 6.5 g. 1-methylpiperazine, and 70 ml. C6H6 kept 5 days at room temp. and the soln. washed and evapd. gave 2.0 g. 10-bromodibenzo[b,f]thiepin (XXVIII), m. 83-4.degree.. The transformation of XXVII into XXVIII was also effected by means of sym-collidine, 2-(Phenylthio)phenylacetic acid (5 g.), 1 g. anhyd. ZnCl2, 7 ml. POCl3, and 2.5 ml. PhNO2 stirred and heated 10 hrs. to 65-70.degree., the mixt. cooled, decompd. with ice, and extd. with C6H6, the ext. washed and distd. with steam, and the residue crystd. from EtOH gave 4.3 g. 10-chlorodibenzo[b,f]thiepin (XXIX), m. 91-3.degree. (cyclohexane-petroleum ether). VIII (3 g.), 5 ml. POCl3, and 0.6 g. ZnCl2 stirred and heated 6 hrs. to 60-70.degree. gave 2.0 g. XXIX, m. 91-2.degree.. VIII (6 g.) in 30 ml. EtOH treated with EtONa (from 0.65 g.

Na and 20 ml. EtOH), the mixt. cooled to 0.degree., stirred and treated with 2.9 g. BuONO, kept 5 hrs. at 0.degree. and 20 hrs. at room temp., dild. with 500 ml. H2O, filtered, and the filtrate acidified with 2N HCl gave 3.6 g. 10,11-dihydrodibenzo[b,f]thiepin-10,11-dione monoxime (XXX), yellow, m. 222-4.degree. (EtOH). XXX (16.7 g.) in 300 ml. tetrahydrofuran reduced with 12.5 g. LiAlH4 in 500 ml. Et2O gave 3.4 g. 11-amino-10,11-dihydrodibenzo[b,f]thiepin-10-ol, m. 195-6.degree. (EtOH); HCl salt monohydrate m. 238-40.degree. (EtOH-Et2O). From the compds. prepd. only IV, X, and XII-XV had significant central depressant activity, none of them exceeding the activity of VII. The pharmacol. data are tabulated.

IT **17037-23-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

=>
=>

=> fil caold
FILE 'CAOLD' ENTERED AT 18:38:05 ON 05 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=>
=>

=> s l10
L16 0 L10

=>
=>

=> fil reg
FILE 'REGISTRY' ENTERED AT 18:38:55 ON 05 DEC 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 DEC 2003 HIGHEST RN 623900-56-1
DICTIONARY FILE UPDATES: 4 DEC 2003 HIGHEST RN 623900-56-1

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

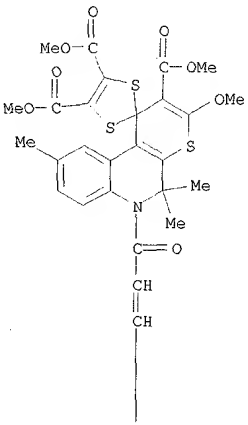
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

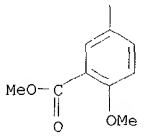
=>
=>

=> d ide can l10 tot

L10 ANSWER 1 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 382652-29-1 REGISTRY
CN Spiro[1,3-dithiole-2,1'-[1H]thiopyrano[2,3-c]quinoline]-2',3',4,5-tetracarboxylic acid, 5',6'-dihydro-6'-[3-[4-methoxy-3-(methoxycarbonyl)phenyl]-1-oxo-2-propenyl]-5',5',9'-trimethyl-, tetramethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C36 H35 N O11 S3
SR Chemical Library
LC STN Files: CHEMCATS

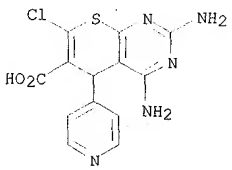
PAGE 1-A





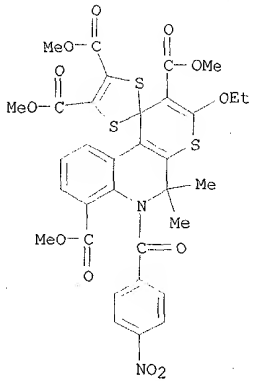
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 2 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 382155-62-6 REGISTRY
CN 5H-Thiopyrano[2,3-d]pyrimidine-6-carboxylic acid, 2,4-diamino-7-chloro-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H10 Cl N5 O2 S
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

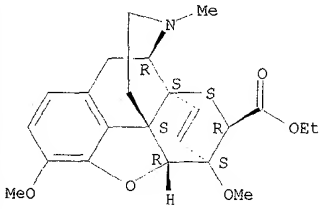
L10 ANSWER 3 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 371948-83-3 REGISTRY
CN Spiro[1,3-dithiole-2,1'-[1H]thiopyrano[2,3-c]quinoline]-2',4,5,7'-tetracarboxylic acid, 3'-ethoxy-5',6'-dihydro-5',5'-dimethyl-6'-(4-nitrobenzoyl)-, tetramethyl ester (9CI) (CA INDEX NAME)
MF C33 H30 N2 O12 S3
SR Chemical Library
LC STN Files: CHEMCATS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L10 ANSWER 4 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 139066-01-6 REGISTRY
CN 4a,7-Etheno-4,12-methano-4aH,6H-benzofuro[3',2':3,4]thiopyrano[2,3-c]pyridine-6-carboxylic acid, 1,2,3,4,7,7a-hexahydro-7,9-dimethoxy-3-methyl-, ethyl ester, [4R-(4.alpha.,4a.alpha.,6.beta.,7.beta.,7a.beta.,12bS*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6,14-Etheno-8-thiamorphinan-7-carboxylic acid, 4,5-epoxy-3,6-dimethoxy-17-methyl-, ethyl ester, (5.alpha.,7.beta.)-
FS STEREOSEARCH
MF C23 H27 N O5 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX
(*File contains numerically searchable property data)

Absolute stereochemistry.



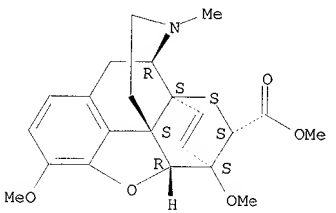
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 116:106551

L10 ANSWER 5 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 138916-19-5 REGISTRY
CN 4a,7-Etheno-4,12-methano-4aH,6H-benzofuro[3',2':3,4]thiopyrano[2,3-c]pyridine-6-carboxylic acid, 1,2,3,4,7,7a-hexahydro-7,9-dimethoxy-3-methyl-, methyl ester, [4R-(4.alpha.,4a.alpha.,6.alpha.,7.beta.,7a.beta.,12bS*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6,14-Etheno-8-thiamorphinan-7-carboxylic acid, 4,5-epoxy-3,6-dimethoxy-17-methyl-, methyl ester, (5.alpha.,7.alpha.)-
FS STEREOSEARCH
MF C22 H25 N O5 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



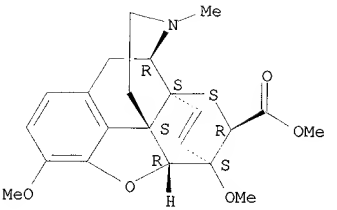
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 116:106551

L10 ANSWER 6 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 138916-18-4 REGISTRY
CN 4a,7-Etheno-4,12-methano-4aH,6H-benzofuro[3',2':3,4]thiopyrano[2,3-c]pyridine-6-carboxylic acid, 1,2,3,4,7,7a-hexahydro-7,9-dimethoxy-3-methyl-, methyl ester, [4R-(4.alpha.,4a.alpha.,6.beta.,7.beta.,7a.beta.,12bS*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6,14-Etheno-8-thiamorphinan-7-carboxylic acid, 4,5-epoxy-3,6-dimethoxy-17-methyl-, methyl ester, (5.alpha.,7.beta.)-
FS STEREOSEARCH
MF C22 H25 N O5 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.



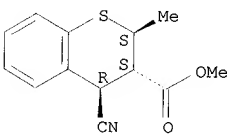
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 116:106551

L10 ANSWER 7 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132747-95-6 REGISTRY
CN 2H-1-Benzothiopyran-3-carboxylic acid, 4-cyano-3,4-dihydro-2-methyl-, methyl ester, (2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H13 N O2 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



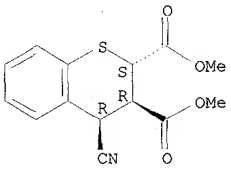
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 8 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132747-94-5 REGISTRY
CN 2H-1-Benzothiopyran-2,3-dicarboxylic acid, 4-cyano-3,4-dihydro-, dimethyl ester, (2.alpha.,3.beta.,4.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C14 H13 N O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



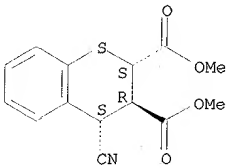
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 9 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132747-93-4 REGISTRY
CN 2H-1-Benzothiopyran-2,3-dicarboxylic acid, 4-cyano-3,4-dihydro-, dimethyl ester, (2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C14 H13 N O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



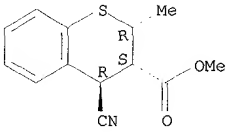
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 10 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132747-92-3 REGISTRY
CN 2H-1-Benzothiopyran-3-carboxylic acid, 4-cyano-3,4-dihydro-2-methyl-, methyl ester, (2.alpha.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H13 N O2 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



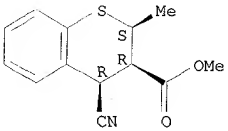
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 11 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132681-57-3 REGISTRY
CN 2H-1-Benzothiopyran-3-carboxylic acid, 4-cyano-3,4-dihydro-2-methyl-, methyl ester, (2.alpha.,3.alpha.,4.alpha.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C13 H13 N O2 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



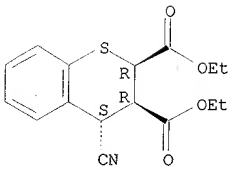
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 12 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132681-56-2 REGISTRY
CN 2H-1-Benzothiopyran-2,3-dicarboxylic acid, 4-cyano-3,4-dihydro-, diethyl ester, (2.alpha.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C16 H17 N O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.



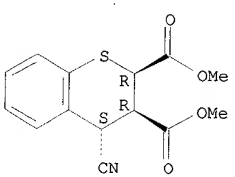
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 13 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN.
RN 132681-55-1 REGISTRY
CN 2H-1-Benzothiopyran-2,3-dicarboxylic acid, 4-cyano-3,4-dihydro-, dimethyl ester, (2.alpha.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C14 H13 N O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Relative stereochemistry.

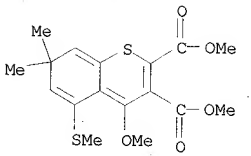


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

L10 ANSWER 14 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 132206-27-0 REGISTRY
CN 7H-1-Benzothiopyran-2,3-dicarboxylic acid, 4-methoxy-7,7-dimethyl-5-(methylthio)-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H20 O5 S2
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



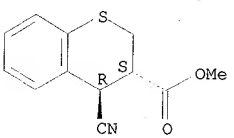
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 115:49581

L10 ANSWER 15 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 120810-24-4 REGISTRY
CN 2H-1-Benzothiopyran-3-carboxylic acid, 4-cyano-3,4-dihydro-, methyl ester, trans- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H11 N O2 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

Relative stereochemistry.



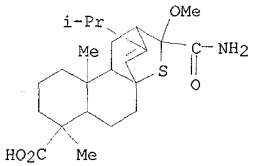
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 114:143072

REFERENCE 2: 110:230939

L10 ANSWER 16 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 108214-21-7 REGISTRY
CN 2,4a-Etheno-4aH-naphtho[2,1-b]thiopyran-7-carboxylic acid, 3-(aminocarbonyl)-1,2,3,5,6,6a,7,8,9,10,10a,10b-dodecahydro-3-methoxy-7,10a-dimethyl-12-(1-methylethyl)-, [2R-(2.alpha.,3.alpha.,4a.alpha.,6a.beta.,7.beta.,10a.alpha.,10b.beta.)]- (9CI) (CA INDEX NAME)
MF C23 H35 N O4 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)

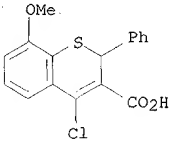


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 107:23538

L10 ANSWER 17 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 99943-65-4 REGISTRY
CN 2H-1-Benzothiopyran-3-carboxylic acid, 4-chloro-8-methoxy-2-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H13 Cl O3 S
SR CA
LC STN Files: CA, CAPLUS, USPATFULL

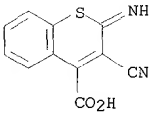


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 104:50730

L10 ANSWER 18 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 99875-39-5 REGISTRY
CN 2H-1-Benzothiopyran-4-carboxylic acid, 3-cyano-2-imino- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H6 N2 O2 S
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)



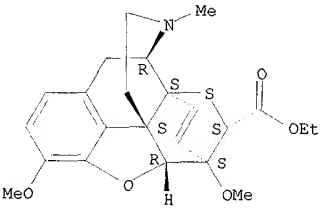
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 104:50757

L10 ANSWER 19 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 87817-36-5 REGISTRY
CN 4a,7-Etheno-4,12-methano-4aH,6H-benzofuro[3',2':3,4]thiopyrano[2,3-c]pyridine-6-carboxylic acid, 1,2,3,4,7,7a-hexahydro-7,9-dimethoxy-3-methyl-, ethyl ester, [4R-(4.alpha.,4a.alpha.,6.alpha.,7.beta.,7a.beta.,12bS*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 6,14-Etheno-8-thiamorphinan-7-carboxylic acid, 4,5-epoxy-3,6-dimethoxy-17-methyl-, ethyl ester, (5.alpha.,7.alpha.)-
FS STEREOSEARCH
MF C23 H27 N O5 S
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

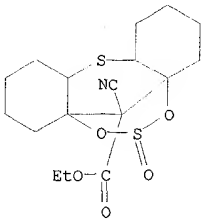
REFERENCE 1: 116:106551

REFERENCE 2: 104:5547

REFERENCE 3: 99:157787

L10 ANSWER 20 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 69695-03-0 REGISTRY
CN 2H,8H-4a,7a-Methanodibenzo[d,g][1,3,2,6]dioxadithiocin-13-carboxylic acid, 13-cyanooctahydro-, ethyl ester, 6-oxide (9CI) (CA INDEX NAME)
FS 3D CONCORD

MF C17 H23 N O5 S2
LC STN Files: CA, CAPLUS, CASREACT

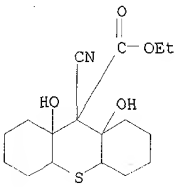


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 90:137783

L10 ANSWER 21 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 69695-02-9 REGISTRY
CN 1H-Thioxanthene-9-carboxylic acid, 9-cyanododecahydro-8a,9a-dihydroxy-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H25 N O4 S
LC STN Files: CA, CAPLUS, CASREACT

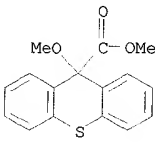


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 90:137783

L10 ANSWER 22 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 57117-06-3 REGISTRY
CN 9H-Thioxanthene-9-carboxylic acid, 9-methoxy-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H14 O3 S
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

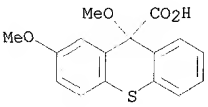


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 83:192270

L10 ANSWER 23 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 43183-19-3 REGISTRY
CN 9H-Thioxanthene-9-carboxylic acid, 2,9-dimethoxy- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H14 O4 S
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

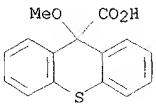


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 79:78739

L10 ANSWER 24 OF 24 REGISTRY COPYRIGHT 2003 ACS on STN
RN 17037-23-9 REGISTRY
CN Thioxanthene-9-carboxylic acid, 9-methoxy- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H12 O3 S
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 68:29676